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Supplemental Material

Within-Day, Between-Day, and Between-Week Variability of Urinary Concentrations of Phenol Biomarkers in Pregnant Women

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Figure S2. Box plots of the distribution of urinary concentrations of 10 phenols (μ g/L, log-scale), creatinine concentration (mg/dL) and specific gravity in within woman weekly-pooled samples from subgroup 1 and subgroup 2 (8 women, n=24 weekly pools, one weekly pool for each of the 3 weeks of collection). Boxes extend from the 25th to the 75th percentile, horizontal bars represent the median, whiskers extend 1.5 times the length of the interquartile range (IQR) above and below the 75th and 25th percentiles, respectively, and outliers are represented as points.

Table S1. Spearman correlation matrix between urinary biomarkers. Each cell outside the diagonal contains the correlations in spot samples (subgroup 1, 2 women, n=114 samples), daily pools (8women, n=56 samples) and weekly pools (8 women, n=24 samples), reported in this order.

Note: The diagonal (highlighted cells and bold font) shows the spearman correlation coefficients for a given biomarker between (*) spot samples and associated daily pools (subgroup 1, 2 women, 114 samples), (§) spot samples and the associated weekly pool (subgroup 1, 2 women, 114 samples) and between (†) daily pools and the associated weekly pool (8 women, 56 samples).

Biomarker	2,4-DCP	2,5-DCP	BP	EP	MP	PP	BP3	BPA	BPS	TCS	Creatinine	Specific gravity
2,4-dichlorophenol	0.36 * 0.20 § 0.63 †											
2,5-dichlorophenol	0.67 0.76 0.47	0.68 * 0.74 § 0.94 †										
Butyl paraben	0.08 0.13 0.39	-0.38 0.01 0.18	0.71 * 0.74 § 0.63 †									
Ethyl paraben	0.11 0.29 0.28	-0.4 0.19 -0.02	0.94 0.55 0.5	0.69 * 0.8 § 0.91 †								
Methyl paraben	0.1 -0.08 0.42	-0.36 -0.39 -0.25	0.58 0.62 0.48	0.62 0.57 0.58	0.70 * 0.62 § 0.87 †							
Propyl paraben	-0.08 -0.27 0.3	-0.51 -0.6 -0.26	0.57 0.5 0.54	0.64 0.08 0.44	0.8 0.69 0.81	0.75 * 0.68 § 0.94 †		_				
Benzophenone-3	0.04 -0.03 -0.29	-0.12 0.32 0.03	0.19 -0.31 -0.09	0.24 0.02 -0.13	0.03 -0.33 -0.34	0.09 -0.54 -0.4	0.11 * 0 § 0.79 †		_			
Bisphenol A	0.5 0.36 0.29	0.1 0.24 0.22	0.24 0.19 0.26	0.33 0.2 0.03	0.28 -0.07 0.14	0.29 -0.19 0	0.15 -0.13 0.05	0.32 * 0.29 § 0.72 †				
Bisphenol S	0.42 -0.01 0.09	0.36 -0.05 -0.28	0.16 0.18 0.33	0.19 0.29 0.05	0.09 0.32 0.43	0.04 0.04 0.24	0.04 -0.03 0.28	0.23 0.08 0.17	0.46 * 0.01 § 0.38 †			
Triclosan	0.53 -0.4 0.23	0.49 -0.5 -0.08	0.14 -0.01 -0.02	0.15 -0.14 0.1	0.13 0.37 0.27	-0.02 0.49 0.42	-0.06 0.1 -0.41	0.26 -0.46 -0.53	0.31 0.15 -0.18	0.43 * 0.09 § 0.82 †		_
Creatinine	0.83 0.46 0.56	0.67 0.34 0.07	0.14 0.51 0.35	0.12 0.19 0.18	0.15 0.2 0.55	-0.06 0.01 0.36	0.05 -0.19 -0.01	0.44 0.61 0.55	0.43 0.22 0.28	0.59 -0.28 -0.15	0.32 * 0.15 § 0.74 †	
Specific gravity	0.79 0.27 0.36	0.67 0.18 0	-0.01 0.62 0.11	-0.02 0.23 0.02	0.03 0.31 0.34	-0.12 0.1 0.13	0.01 -0.19 0.07	0.44 0.49 0.48	0.32 0.3 0.13	0.48 -0.11 -0.14	0.92 0.9 0.86	0.37 * 0.23 § 0.70 †

2,4-DCP = 2,4-dichlorophenol; 2,5-DCP = 2,5-dichlorophenol; BP = butylparaben; EP = ethylparaben; MP = methylparaben; PP = propylparaben; BP3 = benzophenone-3; BPA = bisphenol A; BPS = bisphenol S; TCS = triclosan.

Table S2. Creatinine and specific gravity corrected ICCs – Within-day variability (ICC₁).

Note that ICC_1 is based on log_{10} -transformed creatinine-corrected (ICC_{creat}) and specific gravitycorrected (ICC_{SG}) phenol biomarker concentrations in the unpooled spot samples from subgroup 1 (2 women, n=114 spot samples collected over the first week of collection). Uncorrected ICCs were also reported in bold font to allow for comparison.

	(h	Within-day variability, ICC ₁ based on unpooled spot samples)		
Biomarker	ICC _{uncorrected}	$\frac{\text{Ased on unpooled spot samples)}}{\text{ICC}_{\text{creat}} (95\% \text{ CI})^{b}}$	ICC_{SG} (95% CI) ^c	
Phenols ^a	uncorrected		~~ 、 , ,	
2,4-dichlorophenol	0.12 (0.00, 0.28)	0.05 (0.00, 0.18)	0.12 (0.00, 0.28)	
2,5-dichlorophenol	0.11 (0.00, 0.27)	0.04 (0.00, 0.16)	0.15 (0.00, 0.33)	
Butyl paraben	0.10 (0.00, 0.25)	0.08 (0.00, 0.23)	0.11 (0.00, 0.27)	
Ethyl paraben	0.03 (0.00, 0.15)	0.05 (0.00, 0.18)	0.06 (0.00, 0.20)	
Methyl paraben	0.27 (0.05, 0.49)	0.31 (0.08, 0.53)	0.31 (0.08, 0.54)	
Propyl paraben	0.28 (0.05, 0.50)	0.26 (0.04, 0.48)	0.27 (0.05, 0.49)	
Benzophenone-3	0.26 (0.04, 0.48)	0.31 (0.08, 0.54)	0.27 (0.05, 0.49)	
Bisphenol A	0.21 (0.01, 0.41)	0.26 (0.04, 0.47)	0.25 (0.03, 0.46)	
Bisphenol S	0.50 (0.26, 0.73)	0.49 (0.26, 0.73)	0.55 (0.32, 0.78)	
Triclosan	0.30 (0.08, 0.53)	0.37 (0.14, 0.61)	0.36 (0.12, 0.59)	

ICC: intraclass correlation coefficient

^{*a*} Concentrations <LOD were replaced by instrumental reading values. Instrumental reading values equal to 0 replaced by the non-zero lowest machine value divided by square root of 2.

^b ICCs were estimated from ANOVA model with a random effect on day (14 days), adjusted for creatinine and within-woman meancentering of the data.

^c ICCs were estimated from ANOVA model with a random effect on day (14 days), adjusted for specific gravity and within-woman mean-centering of the data.

Table S3. Random intercept linear mixed models analyses. Within-day (ICC₁), between-day (ICC₂), between-week variability (ICC₃) and alternative estimate of between-week variability based on 3 random spot samples (ICC₄).

Note that ICC_1 , ICC_2 , ICC_3 and ICC_4 are respectively based on log_{10} -transformed phenol biomarker concentrations, creatinine concentration and specific gravity in the unpooled spot samples from subgroup 1 (2 women, n=114 spot samples collected over the first week of collection, ICC_1), in the within woman daily-pooled samples from subgroup 1 and subgroup 2 (8 women, n=56 daily pools, one daily pool for each day of the first week of collection, ICC_2), the within woman weekly-pooled samples from subgroup 1 and subgroup 2 (8 women, n=24 weekly pools, one weekly pool for each of the 3 weeks of collection, ICC_3), the random spot samples from subgroup 1 and subgroup 2 (8 women, n=24 random spot sample, one sample in each of the 3 weeks of collection, ICC_4). Random intercept linear mixed models (maximum likelihood estimates).

	Within-day variability (based on unpooled spot samples)	Between-day variability (based on daily pools)	Between-week variability (based on weekly pools)	Alternative between- week variability (based on three random spot samples)	
Biomarker	$ICC_1 (95\% CI)^b$	ICC ₂ (95% CI) ^c	ICC ₃ (95% CI) ^c	ICC ₄ (95% CI) ^c	
<i>Phenols</i> ^a					
2,4-dichlorophenol	0.11 (0.03, 0.35)	0.90 (0.75, 0.96)	0.61 (0.27, 0.87)	0.45 (0.13, 0.82)	
2,5-dichlorophenol	0.10 (0.02, 0.33)	0.97 (0.93, 0.99)	0.93 (0.78, 0.98)	0.84 (0.59, 0.95)	
Butyl paraben	0.08 (0.01, 0.42)	0.78 (0.53, 0.91)	0.82 (0.57, 0.94)	0.38 (0.09, 0.80)	
Ethyl paraben	NA^d	0.83 (0.62, 0.94)	0.28 (0.04, 0.78)	0.35 (0.07, 0.79)	
Methyl paraben	0.23 (0.09, 0.45)	0.83 (0.61, 0.93)	0.78 (0.50, 0.93)	0.83 (0.57, 0.95)	
Propyl paraben	0.27 (0.11, 0.52)	0.89 (0.73, 0.96)	0.84 (0.60, 0.95)	0.67 (0.33, 0.89)	
Benzophenone-3	0.23 (0.09, 0.47)	0.70 (0.43, 0.88)	0.56 (0.22, 0.85)	0.23 (0.02, 0.79)	
Bisphenol A	0.20 (0.07, 0.45)	0.56 (0.29, 0.81)	0.55 (0.21, 0.85)	0.33 (0.06, 0.79)	
Bisphenol S	0.52 (0.30, 0.73)	0.11 (0.01, 0.55)	0.21 (0.02, 0.80)	0.28 (0.04, 0.78)	
Triclosan	0.28 (0.12, 0.52)	0.88 (0.71, 0.95)	$\mathbf{N}\mathbf{A}^{\mathrm{d}}$	0.05 (0.00, 1.00) ^e	
Urine dilution markers					
Creatinine	0.10 (0.02, 0.32)	0.58 (0.30, 0.82)	0.83 (0.58, 0.95)	0.52 (0.18, 0.84)	
Specific gravity	0.03 (0.00, 0.40)	0.57 (0.29, 0.81)	0.45 (0.13, 0.82)	0.66 (0.32, 0.89)	

ICC: intraclass correlation coefficient, NA: not applicable.

^a Concentrations <LOD were replaced by instrumental reading values. Instrumental reading values equal to 0 replaced by the lowest non-zero machine value divided by square root of 2.

^b ICCs were estimated from random intercept linear mixed model with a random effect on day (14 days) and within-woman mean-centering of the data.

^c ICCs were estimated from random intercept linear mixed model with a random effect on woman.

^d No estimate and confidence interval given by the model due to estimates equal to zero.

^e One sample with extreme value excluded (n=23 samples) for the analysis of triclosan.

Table S4. Random intercept linear mixed models analyses adjusted for creatinine (ICCcreat) or specific gravity (ICC_{SG}) – Within-day variability (ICC₁).

Note that ICC_1 is based on log_{10} -transformed phenol biomarker concentrations in the unpooled spot samples from subgroup 1 (2 women, n=114 spot samples collected over the first week of collection). Models adjusted for creatinine (ICC_{creat}) or specific gravity (ICC_{SG}, maximum likelihood estimates).

	Within-day variability, ICC ₁ (based on unpooled spot samples)					
Biomarker	ICC_{creat} (95% CI) ^b	$ICC_{SG} (95\% \text{ CI})^c$				
Phenols ^a						
2,4-dichlorophenol	0.03 (0.00, 0.81)	0.16 (0.05, 0.42)				
2,5-dichlorophenol	0.11 (0.03, 0.37)	0.20 (0.07, 0.45)				
Butyl paraben	0.06 (0.00, 0.50)	0.08 (0.01, 0.43)				
Ethyl paraben	$\mathbf{N}\mathbf{A}^{\mathrm{d}}$	0.03 (0.00, 0.89)				
Methyl paraben	0.24 (0.10, 0.47)	0.25 (0.11, 0.48)				
Propyl paraben	0.27 (0.11, 0.52)	0.26 (0.11, 0.52)				
Benzophenone-3	0.28 (0.12, 0.52)	0.25 (0.10, 0.49)				
Bisphenol A	0.24 (0.09, 0.50)	0.23 (0.09, 0.49)				
Bisphenol S	0.59 (0.38, 0.78)	0.59 (0.37, 0.78)				
Triclosan	0.34 (0.16, 0.58)	0.34 (0.16, 0.57)				

ICC: intraclass correlation coefficient

^a Concentrations <LOD were replaced by instrumental reading values. Instrumental reading values equal to 0 replaced by the lowest non-zero machine value divided by square root of 2.

^b ICCs were estimated from random intercept linear mixed model with a random effect on day (14 days), adjusted for creatinine and within-woman mean-centering of the data.

^c ICCs were estimated from random intercept linear mixed model with a random effect on day (14 days), adjusted for specific gravity and within-woman mean-centering of the data. ^{*d*} No estimate and confidence interval given by the model due to estimates equal to zero.

Table S5. Creatinine and specific gravity corrected ICCs – Between-day (ICC₂), between-week variability (ICC₃) and alternative estimate of between-week variability based on 3 random spot samples (ICC₄).

Note that ICC₂, ICC₃ and ICC₄ are respectively based on log_{10} -transformed creatinine-corrected (ICC_{creat}) and specific gravity-corrected (ICC_{SG}) phenol biomarker concentrations in the within woman daily-pooled samples from subgroup 1 and subgroup 2 (8 women, n=56 daily pools, one daily pool for each day of the first week of collection, ICC₂), the within woman weekly-pooled samples from subgroup 1 and subgroup 2 (8 women, n=24 weekly pools, one weekly pool for each of the 3 weeks of collection, ICC₃), the random spot samples from subgroup 1 and subgroup 2 (8 women, n=24 random spot samples, one sample in each of the 3 weeks of collection, ICC₄). Models with concentrations corrected for creatinine (ICC_{creat}) or specific gravity (ICC_{SG}). Uncorrected ICCs were also reported in bold font to allow for comparison.

	Between-day variability, ICC ₂			Bet	ween-week variability, I	CC ₃	Alternative between-week variability, ICC ₄		
	(based on daily pools)				(based on weekly pools)		(based on three random spot samples)		
Biomarker	ICCuncorrected	ICC _{creat} (95% CI) ^b	ICC _{SG} (95% CI) ^c	ICCuncorrected	ICC _{creat} (95% CI) ^b	ICC _{SG} (95% CI) ^c	ICCuncorrected	ICC _{creat} (95% CI) ^b	ICC _{SG} (95% CI) ^c
Phenols ^a									
2,4-dichlorophenol	0.91 (0.82, 1.00)	0.94 (0.87, 1.00)	0.94 (0.87, 1.00)	0.65 (0.32, 0.99)	0.55 (0.16, 0.95)	0.58 (0.21, 0.96)	0.50 (0.08, 0.92)	0.44 (0.00, 0.88)	0.52 (0.11, 0.93)
2,5-dichlorophenol	0.98 (0.95, 1.00)	0.98 (0.95, 1.00)	0.98 (0.97, 1.00)	0.93 (0.86, 1.00)	0.93 (0.85, 1.00)	0.93 (0.83, 1.00)	0.85 (0.69, 1.00)	0.83 (0.63, 1.00)	0.89 (0.76, 1.00)
Butyl paraben	0.80 (0.61, 0.99)	0.80 (0.62, 0.99)	0.79 (0.59, 0.98)	0.84 (0.67, 1.00)	0.77 (0.53, 1.00)	0.79 (0.56, 1.00)	0.42 (0.00, 0.87)	0.33 (0.00, 0.80)	0.29 (0.00, 0.76)
Ethyl paraben	0.85 (0.70, 1.00)	0.87 (0.73, 1.00)	0.84 (0.69, 1.00)	0.33 (0.00, 0.79)	0.30 (0.00, 0.76)	0.37 (0.00, 0.83)	0.40 (0.00, 0.85)	0.40 (0.00, 0.85)	0.34 (0.00, 0.80)
Methyl paraben	0.84 (0.69, 1.00)	0.89 (0.78, 1.00)	0.85 (0.70, 1.00)	0.81 (0.60, 1.00)	0.77 (0.53, 1.00)	0.77 (0.52, 1.00)	0.85 (0.68, 1.00)	0.78 (0.55, 1.00)	0.78 (0.54, 1.00)
Propyl paraben	0.90 (0.80, 1.00)	0.91 (0.82, 1.00)	0.90 (0.79, 1.00)	0.86 (0.70, 1.00)	0.85 (0.68, 1.00)	0.84 (0.67, 1.00)	0.70 (0.40, 1.00)	0.60 (0.24, 0.97)	0.63 (0.28, 0.98)
Benzophenone-3	0.73 (0.50, 0.96)	0.75 (0.53, 0.97)	0.75 (0.53, 0.97)	0.60 (0.23, 0.97)	0.62 (0.26, 0.98)	0.60 (0.23, 0.97)	0.28 (0.00, 0.75)	0.38 (0.00, 0.84)	0.31 (0.00, 0.78)
Bisphenol A	0.60 (0.30, 0.89)	0.45 (0.12, 0.78)	0.47 (0.15, 0.79)	0.59 (0.22, 0.97)	0.46 (0.03, 0.90)	0.36 (0.00, 0.82)	0.38 (0.00, 0.83)	$(0.00, 0.42)^{d}$	$(0.00, 0.42)^{d}$
Bisphenol S	0.14 (0.00, 0.39)	0.20 (0.00, 0.48)	0.09 (0.00, 0.31)	0.26 (0.00, 0.73)	0.17 (0.00, 0.64)	0.12 (0.00, 0.57)	0.33 (0.00, 0.80)	0.14 (0.00, 0.60)	0.20 (0.00, 0.68)
Triclosan	0.89 (0.78, 1.00)	0.92 (0.84, 1.00)	0.92 (0.83, 1.00)	$(0.00, 0.44)^{d}$	0.01 (0.00, 0.43)	0.05 (0.00, 0.48)	0.11 (0.00, 0.58)	0.10 (0.00, 0.55)	0.03 (0.00, 0.46)
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ICC: intraclass correlation coefficient.

^a Concentrations <LOD were replaced by instrumental reading values. Instrumental reading values equal to 0 replaced by the lowest non-zero machine value divided by square root of 2.

^b ICCs were estimated from ANOVA model with a random effect on woman and adjusted for creatinine concentration.

^c ICCs were estimated from ANOVA model with a random effect on woman and adjusted for specific gravity.

^d We give only the confidence interval truncated to zero due to negative estimate of ICC.

Table S6. Random intercept linear mixed models analyses adjusted for creatinine (ICC_{creat}) or specific gravity (ICC_{SG}) – Between-day (ICC₂), between-week variability (ICC₃) and alternative estimate of between-week variability based on 3 random spot samples (ICC₄).

Note that ICC_2 , ICC_3 and ICC_4 are respectively based on log_{10} -transformed phenol biomarker concentrations in the within woman daily-pooled samples from subgroup 1 and subgroup 2 (8 women, n=56 daily pools, one daily pool for each day of the first week of collection, ICC_2), the within woman weekly-pooled samples from subgroup 1 and subgroup 2 (8 women, n=24 weekly pools, one weekly pool for each of the 3 weeks of collection, ICC_3), the random spot samples from subgroup 1 and subgroup 2 (8 women, n=24 random spot sample, one sample in each of the 3 weeks of collection, ICC_4). Models adjusted for creatinine (ICC_{creat}) or specific gravity (ICC_{SG} , maximum likelihood estimates).

	Between-day va (based on d	ariability, ICC ₂ laily pools)	Between-week (based on w	variability, ICC ₃ eekly pools)	Alternative between-week variability, ICC ₄ (based on three random spot samples)		
Biomarker	ICC_{creat} (95% CI) ^b	ICC _{SG} (95% CI) ^c	$ICC_{creat} (95\% CI)^{b}$	ICC _{SG} (95% CI) ^c	$ICC_{creat} (95\% \text{ CI})^b$	ICC_{SG} (95% CI) ^c	
Phenols ^a							
2,4-dichlorophenol	0.93 (0.81, 0.97)	0.92 (0.81, 0.97)	0.47 (0.15, 0.83)	0.59 (0.24, 0.87)	0.47 (0.15, 0.82)	0.48 (0.15, 0.83)	
2,5-dichlorophenol	0.98 (0.94, 0.99)	0.98 (0.95, 0.99)	0.92 (0.77, 0.98)	0.93 (0.79, 0.98)	0.83 (0.58, 0.95)	0.90 (0.72, 0.97)	
Butyl paraben	0.78 (0.54, 0.92)	0.76 (0.52, 0.91)	0.94 (0.80, 0.99)	0.86 (0.63, 0.96)	0.34 (0.06, 0.79)	0.25 (0.02, 0.83)	
Ethyl paraben	0.85 (0.66, 0.94)	0.84 (0.64, 0.94)	0.23 (0.02, 0.79)	0.31 (0.05, 0.79)	0.39 (0.09, 0.80)	0.29 (0.04, 0.79)	
Methyl paraben	0.88 (0.72, 0.96)	0.84 (0.63, 0.94)	0.71 (0.35, 0.92)	0.79 (0.50, 0.94)	0.82 (0.54, 0.94)	0.77 (0.43, 0.93)	
Propyl paraben	0.90 (0.75, 0.96)	0.89 (0.73, 0.96)	0.82 (0.54, 0.94)	0.85 (0.62, 0.95)	0.67 (0.32, 0.89)	0.63 (0.27, 0.89)	
Benzophenone-3	0.71 (0.43, 0.88)	0.70 (0.43, 0.88)	0.62 (0.26, 0.89)	0.56 (0.22, 0.85)	0.30 (0.04, 0.81)	0.23 (0.02, 0.79)	
Bisphenol A	0.44 (0.18, 0.73)	0.50 (0.23, 0.77)	0.45 (0.13, 0.81)	0.50 (0.15, 0.85)	NA^d	\mathbf{NA}^{d}	
Bisphenol S	0.11 (0.01, 0.55)	0.07 (0.00, 0.62)	0.12 (0.00, 0.89)	0.25 (0.02, 0.87)	0.12 (0.00, 0.92)	0.21 (0.02, 0.80)	
Triclosan	0.90 (0.74, 0.96)	0.90 (0.75, 0.96)	NA ^d	NA ^d	$0.23 (0.02, 0.85)^{e}$	$0.07 (0.00, 0.99)^{e}$	

ICC: intraclass correlation coefficient, NA: not applicable.

^a Concentrations <LOD were replaced by instrumental reading values. Instrumental reading values equal to 0 replaced by the lowest non-zero machine value divided by square root of 2.

^a ICCs were estimated from random intercept linear mixed model with a random effect on woman and adjusted for creatinine concentration.

^b ICCs were estimated from random intercept linear mixed model with a random effect on woman and adjusted for specific gravity.

^d No estimate and confidence interval given by the model due to estimates equal to zero.

^e One sample with extreme value excluded (n=23 samples) for the analysis of triclosan.

Figure S1. Box plots of the distribution of urinary concentrations of 10 phenols (μ g/L, log-scale), creatinine concentration (mg/dL) and specific gravity in the within woman daily-pooled samples from subgroup 1 and subgroup 2 (8 women, n=56 daily pools, one daily pool for each day of the first week of collection). Boxes extend from the 25th to the 75th percentile, horizontal bars represent the median, whiskers extend 1.5 times the length of the interquartile range (IQR) above and below the 75th and 25th percentiles, respectively, and outliers are represented as points.

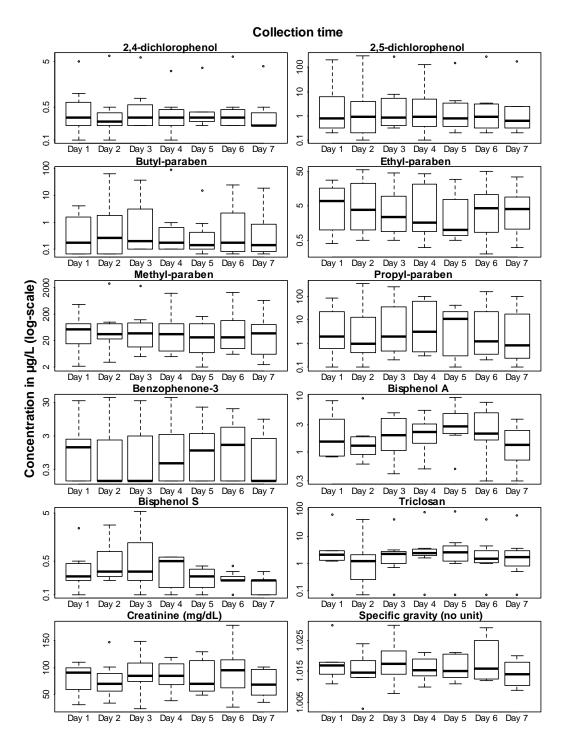


Figure S2. Box plots of the distribution of urinary concentrations of 10 phenols (μ g/L, log-scale), creatinine concentration (mg/dL) and specific gravity in within woman weekly-pooled samples from subgroup 1 and subgroup 2 (8 women, n=24 weekly pools, one weekly pool for each of the 3 weeks of collection). Boxes extend from the 25th to the 75th percentile, horizontal bars represent the median, whiskers extend 1.5 times the length of the interquartile range (IQR) above and below the 75th and 25th percentiles, respectively, and outliers are represented as points.

